Electronic Supplementary information for

In Silico Interactome of a Room-Temperature Ferroelectric Nematic Material

Richard J. Mandle [1,2]

[1] School of Physics and Astronomy, University of Leeds, Leeds LS2 9JT, UK; r.mandle@leeds.ac.uk
[2] School of Chemistry, University of Leeds, Leeds LS2 9HT, UK

Table S1. Orientational order parameter (<*P*2>) and simulation density (g cm^3) as a function of temperature for simulations beginning from an isotropic initial configuration. Regardless of the temperature employed, nematic order fails to spontaneously emerge.

T / K	<*P*2>	Density g cm^3
278	0.06±0.012	1.34±0.002
288	0.03±0.008	1.34±0.003
298	0.06±0.010	1.33±0.004
308	0.06±0.010	1.33±0.004
318	0.06±0.005	1.32±0.004
328	0.07±0.005	1.31±0.003
338	0.07±0.005	1.30±0.003
348	0.07±0.005	1.29±0.002
358	0.06±0.004	1.29±0.003

Table S2. Tabulated data for key properties of atomistic simulations of UUQU-4-N beginning in a **polar** nematic configuration.

T / K	<*P*1>	<*P*2>	<*B*>	Ps / C.m^2	Density/ kg m^3
258	0.952 ±0.001	0.721 ±0.005	0.006 ±0.003	0.059 ±0.01	1365 ±1.597
268	0.948 ±0.001	0.701 ±0.005	0.014 ±0.004	0.059 ±0.01	1363 ±1.867
278	0.934 ±0.001	0.681 ±0.004	0.006 ±0.003	0.058 ±0.01	1355 ±1.797
288	0.929 ±0.001	0.671 ±0.006	0.008 ±0.004	0.057 ±0.01	1348 ±2.029
298	0.899 ±0.002	0.622 ±0.007	0.011 ±0.005	0.055 ±0.01	1334 ±2.08
308	0.853 ±0.005	0.564 ±0.01	0.016 ±0.007	0.051 ±0.01	1325 ±2.164
318	0.593 ±0.01	0.363 ±0.012	0.021 ±0.011	0.035 ±0.01	1308 ±2.211
328	0.102 ±0.011	0.082 ±0.022	0.061 ±0.02	0.006 ±0.01	1298 ±2.347
338	0.017 ±0.008	0.072 ±0.011	0.068 ±0.021	0.001 ±0.01	1287 ±2.46
348	0.035 ±0.009	0.085 ±0.018	0.034 ±0.016	0.002 ±0.01	1277 ±2.653

We performed an MD simulation beginning from an apolar pseudo nematic starting configuration of UUQU-4-N by having a 1:1 mixture of molecules oriented with their long axis along either the x+ or x- directions. During the subsequent production MD simulation the nematic order parameter steadily decays towards zero, and the simulation was stopped at around 80 nanoseconds (Figure S1). The polar order parameter <*P*1> is near zero during the entire simulation.

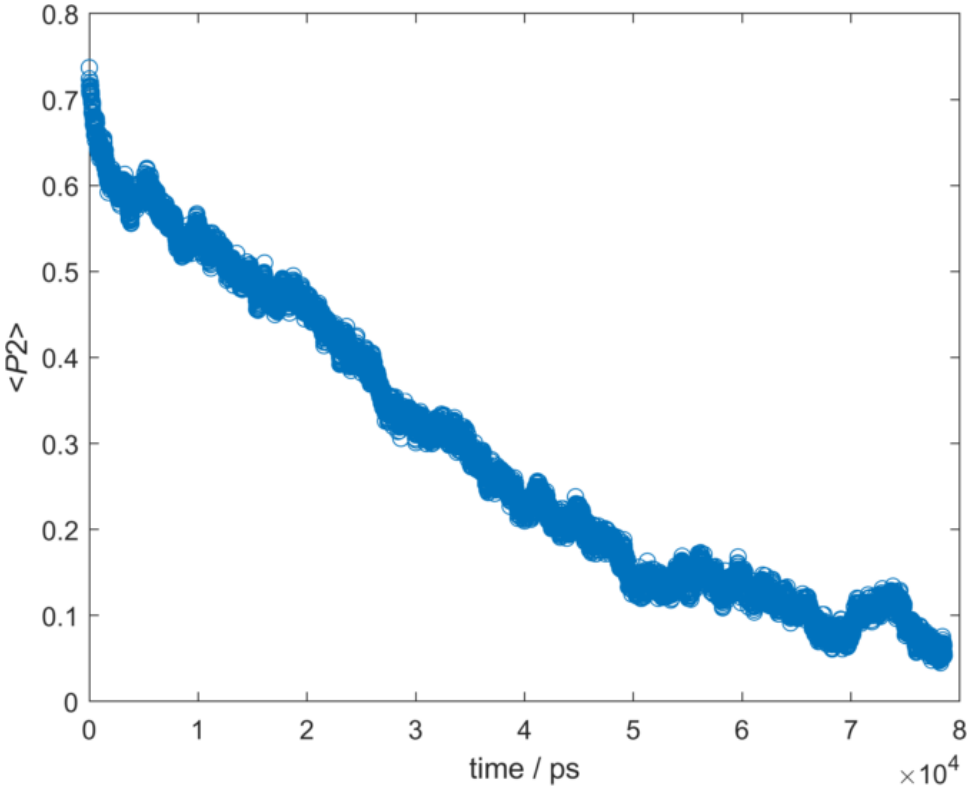

Figure S1. Plot of <*P*2> as a function of simulation time (ps) for an MD simulation of UUQU-4-N beginning from a pseudo nematic starting configuration at a temperature of 288 K.

Calculation of CDF

The cylindrical distribution function (CDF) is calculated as outlined in Figure S2. All operations are performed over each frame in the production simulation. The CDF is computed for a reference set of positions, in this case the molecular centre of mass. For all molecules within the simulation we look for neighbouring positions using cylindrical shells, with the height (*h*) of these shells being oriented parallel to the nematic director (n) in each frame. The number of counts within each shell is normalized against the shell volume and the average density, giving the CDF plots shown. We use a cylinder length cut-off of +/- 40 Å, a radius cut-off of 15 Å, and a step-size of 0.04 Å for each shell size increment (Δh, Δr).

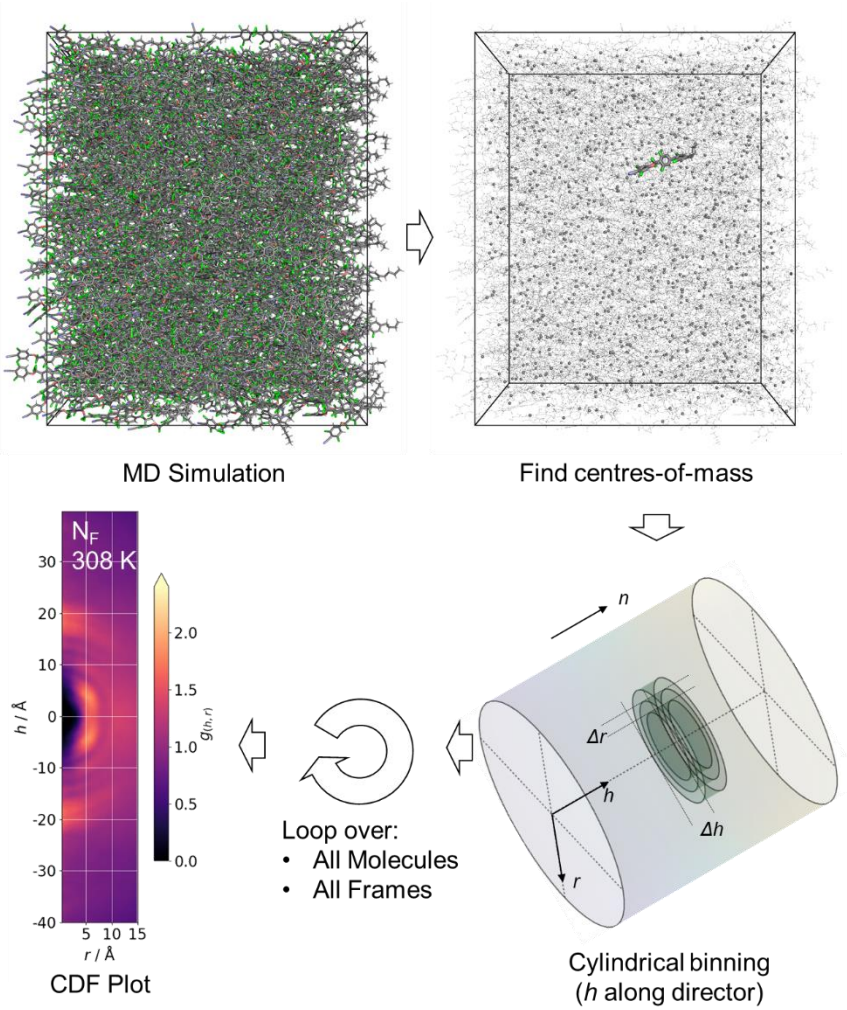

Figure S2. Schematic overview of the CDF process.

As described in the manuscript, a simulated electric field is used to generate the polar nematic configuration. We computed the CDF for the N_F phase of UUQU-4-N at 308K, but for 20 nanosecond wide “windows” rather than doing so for all frames. The resulting CDF plots are, to a first approximation identical, indicating that the pairing modes are preserved independently of the field used to generate the initial configuration.

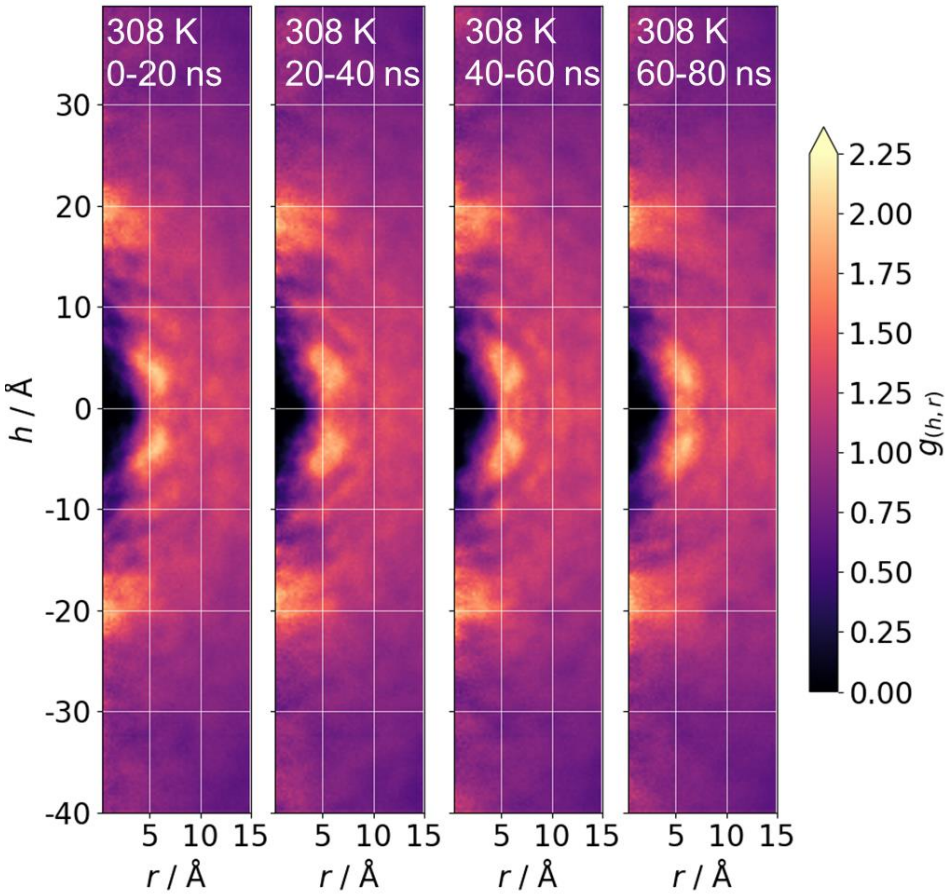

Figure S3. Evolution of the CDF over time.